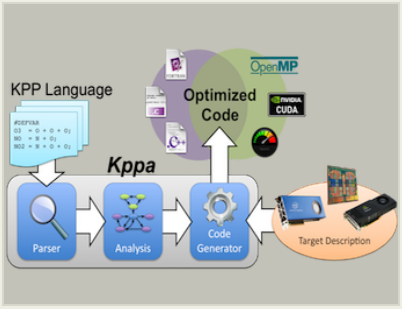
Operational High Resolution Chemical Kinetics Simulation, Phase I

Completed Technology Project (2017 - 2017)

Project Introduction

Numerical simulations of chemical kinetics are critical to addressing urgent issues in both the developed and developing world. Ongoing demand for higher resolution models with larger chemical mechanisms drives exponential growth in computational cost: many models spend over 90% of their runtime simulating chemical kinetics. Energy efficiency and renewable energy system research and development depend on simulations involving thousands of chemical species and reactions, but there are no general analysis tools that can handle mechanisms of this size. Simulations of more than a few hundred species or reactions are hand-tuned, ad-hoc solutions that will ultimately become obsolete. ParaTools will address this need by improving its "Kppa" general analysis tool for chemical kinetics to facilitate coupling with high resolution models and to support large chemical mechanisms. Phase I will explore the feasibility of methods for large mechanism support including flux analysis for sub-cell parallelization and mechanism reduction, dynamic mechanism selection based on environmental conditions, and iterative methods for large sparse systems. Phase I will also improve Kppa as a general analysis source code generator by implementing accelerated analysis methods that use many-core and multi-core devices and/or GPUs to reduce mechanism analysis, support for non-Arrhenius reaction rates, and an interface for coupling Kppa-generated code with high resolution models. Phase II will implement large mechanism support based on Phase I findings. Pre-coupled open source model packages containing Kppa-generated source coupled with a multi-physics or flow code will be provided in Phase I to facilitate commercialization through Phase II and beyond. The improved Kppa tool will reduce time-to-solution by combining the latest numerical and algorithmic developments with accelerated computing technology to enable supercomputer-level performance on smaller computers with lower costs.



Operational High Resolution Chemical Kinetics Simulation, Phase I Briefing Chart Image

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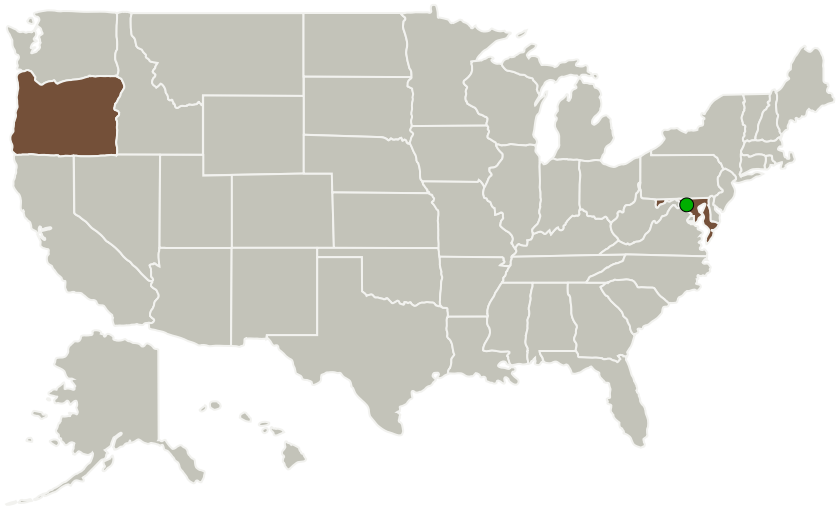
Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
ParaTools, Inc.	Lead Organization	Industry	Eugene, Oregon
Goddard Space Flight Center(GSFC)	Supporting Organization	NASA Center	Greenbelt, Maryland

Primary U.S. Work Locations	
Maryland	Oregon

Organizational Responsibility

Responsible Mission Directorate:

Space Technology Mission Directorate (STMD)

Lead Organization:

ParaTools, Inc.

Responsible Program:

Small Business Innovation Research/Small Business Tech Transfer

Project Management

Program Director:

Jason L Kessler

Program Manager:

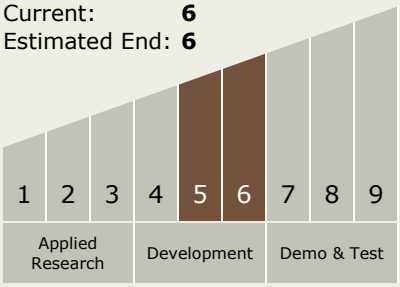
Carlos Torrez

Principal Investigator:

John C Linford

Technology Maturity (TRL)

Start: **5**
Current: **6**
Estimated End: **6**



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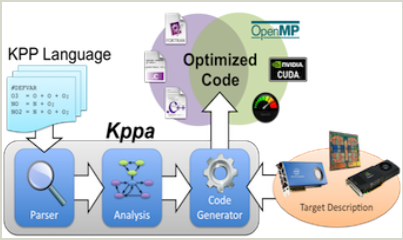
Images



Briefing Chart Image
Operational High Resolution Chemical Kinetics Simulation, Phase I Briefing Chart Image *(https://techport.nasa.gov/image/132342)*

Technology Areas

Primary:

- TX11 Software, Modeling, Simulation, and Information Processing
  - TX11.6 Ground Computing
    - TX11.6.7 High Performance Data Analytics Platform

Target Destinations

The Sun, Earth, The Moon, Mars, Others Inside the Solar System, Outside the Solar System